



The High-Fidelity Generalized Method of Cells with arbitrary cell geometry and its relationship to the Parametric Finite-Volume Micromechanics

Marcio A.A. Cavalcante^a, Eduardo N. Lages^b, Severino P.C. Marques^b, Marek-Jerzy Pindera^{a,*}

^a Civil and Environmental Engineering Department, University of Virginia, Charlottesville, VA 22904-4742, USA

^b Center of Technology, Federal University of Alagoas, Maceio, Alagoas, Brazil

ARTICLE INFO

Article history:

Received 10 February 2011

Received in revised form 30 March 2012

Available online 19 April 2012

Keywords:

Finite-volume theory

Homogenization

Micromechanics

Parametric mapping

ABSTRACT

This contribution is motivated by the recent IJSS article titled “Formulation of the High-Fidelity Generalized Method of Cells with Arbitrary Cell Geometry for Refined Micromechanics and Damage in Composites” by Haj-Ali and Aboudi. In the present discussion, we critically compare these authors’ approach with the Parametric Finite-Volume Direct Averaging Micromechanics (FVDAM) theory developed in a sequence of papers dating to 2004. We show that the extension proposed by Haj-Ali and Aboudi follows the framework of the parametric FVDAM theory, and not the original HFGMC model as claimed. Just as importantly, we demonstrate that the proposed extension is fundamentally flawed as it violates accepted principles which every mechanics theory must satisfy, namely correct reducibility and coordinate frame indifference. Direct comparison of predictions generated by the parametric FVDAM theory, the proposed extension called HFGMC with arbitrary cell geometry and finite-element method demonstrates no need for the extension carried out in the specific manner proposed by Haj-Ali and Aboudi, which in fact produces inferior results.

© 2012 Elsevier Ltd. All rights reserved.

1. Introduction

The Higher-Order Theory for Functionally Graded Materials (HOTFGM), developed in a sequence of papers in the 1990’s and summarized in Aboudi et al. (1999), provided the main framework for the construction of its homogenized counterpart initially named the higher-order theory for periodic multiphase materials by Aboudi et al. (2001). The homogenized version was subsequently renamed the High-Fidelity Generalized Method of Cells (HFGMC) by Aboudi et al. (2002) despite the fact that predictions of HFGMC generally do not reduce to those of the Generalized Method of Cells (GMC) (Paley and Aboudi, 1992), as expected of theories related to each other through similar names. Both HOTFGM and so-called HFGMC are based on the discretization of a functionally graded or periodic material microstructure into **rectangular** generic cells which are further subdivided into four or eight subcells, depending on the investigated problem’s dimensionality. An incomplete quadratic displacement field representation is employed in each subcell, characterized by unknown coefficients which are determined by satisfying different moments of the equilibrium equations in a volume-average sense, and continuity of displacement and tractions between individual subcells

within generic cells and between generic cells in a surface-average sense, following the original idea proposed by Achenbach (1975).

Both HOTFGM and HFGMC theories have been substantially reconstructed in a sequence of papers by Bansal and Pindera (2003, 2005, 2006) and Zhong et al. (2004) using domain discretization based solely on single rectangular subvolumes, the same incomplete displacement field representation within each subvolume as in the original higher-order approaches, satisfaction of the equilibrium equations in a surface-averaged sense (without the need for the higher-order moments), and imposition of traction and displacement continuity between adjacent subvolumes in a surface-average sense. The surface-averaging character of the reconstructed theories made possible the implementation of the local–global stiffness matrix approach which, in turn, facilitated comparison with the finite-element approaches used to solve the same classes of problems. The significant re-constructions had tremendously simplified the theoretical framework of both techniques and, more importantly, demonstrated that they belong to the class of techniques called finite-volume methods which have gained popularity in the solution of solid mechanics problems in the past 20 years, thereby providing a rational basis for the second name change *finite-volume direct averaging micromechanics* (FVDAM) in the case of HFGMC. Table 1 compares the features of the original HFGMC and FVDAM theories based on rectangular discretizations.

The defining feature of the finite-volume techniques, originally developed for fluid mechanics problems (cf. Versteeg and

* Corresponding author.

E-mail address: mp3g@virginia.edu (M.-J. Pindera).

Table 1
Comparison of the features of the original higher-order theory for periodic multiphase materials, Aboudi et al. (2001), subsequently renamed HFGMC by Aboudi et al. (2002), and FVDAM models. The highlighted entries in the middle and right columns denote differences in the corresponding features listed in the left column.

Feature	HFGMC	FVDAM
Unit cell discretization	Generic cells with 4 subcells	Single subvolumes
Subdomain geometry	Rectangular generic cells/subcells	Rectangular subvolumes
Displacement field	Quadratic in local coordinates without cross-product terms	Quadratic in local coordinates without cross-product terms
Variables	Moments of volume-averaged subcell stresses; displacement field microvariables	Surface-averaged subvolume interfacial tractions and displacements
Equilibrium equations	0th, 1st and 2nd moments satisfied in volume-average sense in each subcell	Satisfied directly in surface-average sense in each subvolume
Continuity conditions (after Achenbach (1975))	Subcell/generic cell interfacial tractions and displacements satisfied in surface-average sense	Subvolume interfacial tractions and displacements satisfied in surface-average sense
Solution technique	Standard assembly	Local/global stiffness matrix

Malalasekera, 1995), is the direct satisfaction of local field equations within control subvolumes q of a discretized domain in a volume-average sense, which for elasticity-type problems reduces to the equilibrium equations,

$$\int_{V(q)} \left(\frac{\partial \sigma_{ji}}{\partial x_j} + F_i \right) dV_{(q)} = 0$$

Starting with the work of Demirdzic et al. (1988), Fryer et al. (1991), Demirdzic and Martinovic (1993), Demirdzic and Muzaferija (1994), Bailey and Cross (1995), Taylor et al. (1995) and Wheel (1996), the applications and further development of this technique continue, characterized by differences in the domain discretization, subvolume displacement field representations (using shape functions borrowed from the finite-element method), and manner of defining control subvolumes used in satisfying the local equilibrium equations, cf. Taylor et al. (2003), Wenke and Wheel (2003), Fallah (2004, 2005a,b, 2006). New applications are continuously sought, including large-deformation extrusion problems (Basic et al., 2005), incompressible and micropolar elasticity problems (Bijelonja et al., 2006; Wheel, 2008).

In the IJSS article titled “Formulation of the High-Fidelity Generalized Method of Cells with Arbitrary Cell Geometry for Refined Micromechanics and Damage in Composites” (Haj-Ali and Aboudi, 2010), the authors claim to introduce two new enhancements into the High-Fidelity Generalized Method of Cells model. The first enhancement is the incorporation of parametric mapping in order to enable the use of quadrilateral subvolumes in simulating the microstructure of periodic heterogeneous materials with greater fidelity relative to the version based on rectangular generic cell and subcell discretization employed in the original model of Aboudi et al. (2001, 2002). The use of parametric mapping is presented as their own without referencing the original idea first introduced by Cavalcante (2006) into the reconstructed framework of the finite-volume theory for functionally graded materials of Bansal and Pindera (2003), and subsequently published in a sequence of papers (Cavalcante et al., 2007a,b, 2008, 2009). This parametric mapping, together with its characteristic simplification, was later adopted to enhance the original version of the FVDAM theory based on rectangular subvolume discretization of a unit cell in a sequence of papers by Gattu et al. (2008), Khatam and Pindera (2009a,b, 2010, 2011) and Khatam et al. (2009), which was subsequently renamed parametric FVDAM. We note that independent of the above finite-volume approaches to the analysis of functionally graded and periodic materials, parametric mapping was also introduced by Fallah (2005a, 2006) into the cell-centered finite-volume formulation of the Mindlin-Reissner plate theory, and by Fallah (2005b, 2008) into two-dimensional stress analysis of solids, which Haj-Ali and Aboudi (2010) also do not reference. While the parametric mapping employed by Fallah (2006) contains no simplifications, the mapping proposed by Cavalcante (2006) employs the concept of volume-average Jacobian as its defining feature consistent with the

surface-averaging framework of the parametric finite-volume theory. Quadrilateral subvolumes were also introduced into the original FVDAM framework by Gao et al. (2009) based on direct geometric (rather than parametric mapping) approach.

The second enhancement proposed by Haj-Ali and Aboudi (2010) is the addition of cross-product terms to the quadratic representation of the fluctuating displacement field within individual subvolumes of the discretized unit cell microstructure in order to render it complete. This enhancement was initially suggested by Cavalcante et al. (2008) as a means of improving the non-traction stress components at the subvolume level, but not carried out in the manner proposed by Haj-Ali and Aboudi (2010) for reasons that will become clear later. We note that the complete quadratic polynomial approximation of subvolume displacement field which includes cross-product terms was successfully employed by Pan et al. (2010) for **triangular subvolumes** in the context of the vertex-based finite-volume method. Introduction of such terms into a finite-volume theory based on **quadrilateral subvolumes** and the surface-averaging approach requires much care, and may potentially lead to problems if done in an ad hoc manner using additional equations lacking physical meaning.

In light of the above overview of the FVDAM theory's evolution, the purpose of this communication is to: critically examine similarities and differences between the parametric FVDAM and HFGMC models; point out fundamental flaws in the authors' proposed approach which may lead to problems encountered by potential users of this method; and lastly clarify misstatements and highlight omissions by Haj-Ali and Aboudi about the standard and parametric FVDAM theories.

The paper is organized as follows. In Section 2 we compare the FVDAM and HFGMC approaches with parametric mapping capabilities which enable efficient reproduction of a heterogeneous material's microstructure with high resolution, summarizing in tabular form similarities and differences. Section 3 discusses the fundamental flaws in the proposed extension's construction which may lead to the violation of accepted mechanics principles, including coordinate frame indifference, in contrast with the self-consistency and completeness of the parametric FVDAM theory's framework. Examples are presented that highlight the problems that a potential user of the extension proposed by Haj-Ali and Aboudi (2010) may encounter. In order to verify Haj-Ali and Aboudi's unsubstantiated claim for the need to include cross-product terms, we incorporate these terms into the displacement field representation used in the parametric FVDAM theory, together with the related additional equations, and compare the predictive capability of both approaches in Section 4. Direct comparison with the finite-element method is also included using virtually the same unit cell discretizations, similar displacement field approximations and a recently introduced stress measure (Cavalcante et al., 2011). In Section 5 we briefly discuss the circumstances under which name changes of proposed theories are justified. Finally, the conclusions that logically follow from the presented evidence are given in Section 6.

2. Parametric FVDAM and HFGMC models

In this section we show that the HFGMC model with parametric mapping capability proposed by Haj-Ali and Aboudi (2010) is in fact based on the FVDAM framework, and not on the original higher-order theory for periodic multiphase materials developed by Aboudi et al. (2001) and subsequently renamed HFGMC by Aboudi et al. (2002). Table 2 compares the basic features of the parametric FVDAM and HFGMC models for quick reference, discussed in detail below.

Both the parametric FVDAM and HFGMC models use the 0th order homogenization theory wherein the displacement field in the q th subdomain of the unit cell is represented in terms of two-scale expansion involving macroscopic and microstructure-induced fluctuating components,

$$u_i^{(q)} = \bar{\varepsilon}_{ij}x_j + u_i^{(q)}, \quad (i = 1, 2, 3). \quad (1)$$

In the above, $\bar{\varepsilon}_{ij}$ are the specified macroscopic or average strains applied to the entire material, and thus the unit cell. In both models, the unit cell is discretized into quadrilateral subvolumes (q) generated from a reference square subvolume using auxiliary parametric coordinates.

In the parametric FVDAM theory, the location of the q th quadrilateral subvolume in the actual microstructure is defined by the vertices ($y_2^{(p,q)}, y_3^{(p,q)}$) referred to a **fixed** coordinate system, in contrast with the original HFGMC model based on two-level discretization into generic cells and subcells. The location of the fixed coordinate system is immaterial since the parametric FVDAM theory obeys the coordinate frame indifference principle. The q th subvolume is an image of the reference subvolume in the $\eta - \xi$ plane bounded by $-1 \leq \eta \leq +1$ and $-1 \leq \xi \leq +1$, Fig. 1. Its vertices correspond to the vertices of the q th subvolume in the actual microstructure. In the parametric FVDAM theory, the mapping of the point (η, ξ) to the corresponding point in the q th subvolume is given by $y_i^{(q)}(\eta, \xi) = \sum_{p=1}^4 N_p(\eta, \xi) y_i^{(p,q)}$ ($i = 2, 3$) where

$$\begin{aligned} N_1(\eta, \xi) &= \frac{1}{4}(1 - \eta)(1 - \xi), & N_2(\eta, \xi) &= \frac{1}{4}(1 + \eta)(1 - \xi), \\ N_3(\eta, \xi) &= \frac{1}{4}(1 + \eta)(1 + \xi), & N_4(\eta, \xi) &= \frac{1}{4}(1 - \eta)(1 + \xi). \end{aligned} \quad (2)$$

This is the same mapping as that employed for the Q4 element which ensures that the sides of the mapped element remain straight. This mapping was originally introduced into the structural version of the finite-volume theory (for functionally graded materials) by Cavalcante (2006), and subsequently used in a sequence of papers cited in the Introduction to solve a variety of problems.

Haj-Ali and Aboudi (2010) also use the same mapping with the coordinates (η, ξ) replaced by (r, s) , following the notation

employed by Fallah (2006). However, the important distinction is that the mapping is defined with respect to **local** coordinate systems centered within each subvolume wherein the quadrilateral subvolume vertices are defined. In Haj-Ali and Aboudi's extension of the parametric FVDAM theory, the choice of the coordinate system that defines the parametric mapping plays a critical role which will be discussed later, rendering it coordinate frame dependent in contrast with the already established theory.

In the parametric FVDAM theory, the fluctuating displacement components in the q th subvolume are given in terms of the reference subvolume coordinates (η, ξ) ,

$$u_i^{(q)} = W_{i(00)}^{(q)} + \eta W_{i(10)}^{(q)} + \xi W_{i(01)}^{(q)} + \frac{1}{2}(3\eta^2 - 1)W_{i(20)}^{(q)} + \frac{1}{2}(3\xi^2 - 1)W_{i(02)}^{(q)} \quad (3)$$

and not in terms of the physical subcell coordinates (y_2, y_3) as incorrectly stated by Haj-Ali and Aboudi, in contrast with the original FVDAM theory based on rectangular unit cell discretization. The same form is used for the actual displacement components in the structural version of the theory. There are 10 and 15 unknown coefficients $W_{i(-)}^{(q)}$ for plane stress and generalized plane strain problems, respectively. In contrast with the nodal-based displacement representation used in finite-element analyses or vertex-based finite-volume theories (Fallah, 2004), cross-product terms are not necessary due to the employed surface-averaging approach in satisfying equilibrium equations, and interfacial traction/displacement continuity and periodicity conditions. The unknown coefficients $W_{i(-)}^{(q)}$ are obtained in terms of the surface-averaged fluctuating displacements

$$\hat{u}_i^{(1,3)} = \frac{1}{2} \int_{-1}^{+1} u_i'(\eta, \mp 1) d\eta, \quad \hat{u}_i^{(2,4)} = \frac{1}{2} \int_{-1}^{+1} u_i'(\pm 1, \xi) d\xi, \quad (4)$$

upon satisfaction of the equilibrium equations in the integral sense in each subvolume (assuming absence of body forces),

$$\int_{V(q)} \frac{\partial \sigma_{ji}}{\partial x_j} dV_{(q)} = \int_{S(q)} t_i^{(q)} dS_{(q)} = \int_{S(q)} \sigma_{ji}^{(q)} n_j^{(q)} dS_{(q)} = 0. \quad (5)$$

As mentioned in the Introduction, direct satisfaction of the equilibrium equations in the integral sense is the distinguishing feature of the different variants of the finite-volume theories, setting it apart from the variational-based finite-element techniques.

A key simplification exploited in the FVDAM theory, which is one of its defining features, is the use of volume-averaged Jacobian $\bar{\mathbf{J}}$ in the relations between surface-averaged displacement gradients on the faces of the q th subvolume in the reference and actual coordinate systems,

Table 2

Comparison of the features of the proposed HFGMC with quadrilateral cells and the parametric FVDAM theory. The highlighted entries in the middle and right columns denote differences in the corresponding features listed in the left column.

Feature	Quadrilateral Cell HFGMC	Parametric FVDAM
Unit cell discretization	Single subcells ^a	Single subvolumes
Subdomain geometry	Quadrilateral by parametric mapping ^c	Quadrilateral by parametric mapping ^b
Displacement field	Quadratic in reference coordinates with cross-product terms	Quadratic in reference coordinates without cross-product terms
Variables	Displacement field coefficients	Surface-averaged interfacial tractions & displacements
Equilibrium equations	Satisfied in surface-average sense	Satisfied in surface-average sense
Moment equations	Satisfied in volume-average sense	Not necessary
Continuity conditions (after Achenbach (1975))	Interfacial tractions/displacements applied in surface-average sense	Interfacial tractions/displacements applied in surface-average sense
Solution technique	Standard assembly	Local/global stiffness matrix

^a Following Bansal and Pindera (2003, 2005) and Gattu et al. (2008), and NOT the original construction of the higher-order theory for periodic materials, (Aboudi et al., 2001), subsequently renamed HFGMC by Aboudi et al. (2002)

^b Originally introduced by Cavalcante (2006) into the re-constructed finite-volume theory for functionally graded materials by Bansal and Pindera (2003)

^c Introduced as original idea by Haj-Ali and Aboudi (2010)

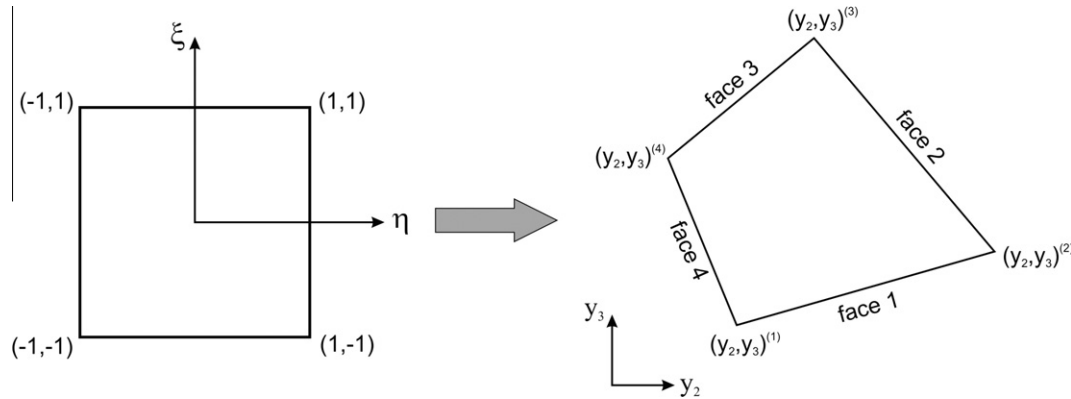


Fig. 1. Mapping of the reference square subvolume in the $\eta - \xi$ coordinate system onto the corresponding quadrilateral subvolume in the actual microstructure defined in the $y_2 - y_3$ coordinate system introduced for the first time by Cavalcante (2006) in the context of the structural version of the parametric finite-volume theory for functionally graded materials, and subsequently incorporated into the parametric FVDAM theory by Gattu et al. (2008).

$$\begin{bmatrix} \frac{\partial u_i}{\partial y_2} \\ \frac{\partial u_i}{\partial y_3} \end{bmatrix}^{(p)} = \hat{\mathbf{J}} \begin{bmatrix} \frac{\partial u_i}{\partial \eta} \\ \frac{\partial u_i}{\partial \xi} \end{bmatrix}^{(\hat{p})} \quad \text{where } \hat{\mathbf{J}}^{-1} = \hat{\mathbf{J}} = \frac{1}{4} \int_{-1}^{+1} \int_{-1}^{+1} \mathbf{J} d\eta d\xi \quad (6)$$

where p and \hat{p} denote the faces of quadrilateral and reference subvolumes, respectively, with $\hat{p} = 1, 3 \rightarrow \xi = \mp 1$ and $\hat{p} = 2, 4 \rightarrow \eta = \pm 1$. The above simplification, originally proposed by Cavalcante (2006) in the context of the finite-volume theory for functionally graded materials, serves two purposes. First, it ensures consistent averaging of the local stress fields based on the use of either surface or volume integrals in the average stress theorem. Second, it enables derivation of explicit expressions for the elements of the local stiffness matrix for the q th subvolume, which relates surface-averaged traction and fluctuating displacement components, given directly in terms of the subvolume geometry and material parameters. The local stiffness matrix formulation enables efficient enforcement of interfacial traction and displacement continuity conditions which, in conjunction with the periodicity conditions, produce solution for the surface-averaged displacements in terms of the applied homogenized strain components $\bar{\varepsilon}_{ij}$, thereby yielding the homogenized elastic properties. Haj-Ali and Aboudi (2010) erroneously refer to the above local/global stiffness matrix approach as condensation. We note that the use of variable Jacobian presents no fundamental difficulties, but does require numerical integration of certain terms in the expressions for local stiffness matrix elements as in the finite-element approach. This slows down considerably the global stiffness matrix assembly (Cavalcante et al., 2008), which is one of the motivation for the approximation used in Eq. (6).

In contrast with the above self-contained, and internally consistent formulation, Haj-Ali and Aboudi introduce cross-product terms into the fluctuating displacement field representation employed in the parametric FVDAM theory, Eq. (3),

$$u_i^{(q)} = W_{i(00)}^{(q)} + \eta W_{i(10)}^{(q)} + \xi W_{i(01)}^{(q)} + \eta \xi W_{i(11)}^{(q)} + \frac{1}{2}(3\eta^2 - 1)W_{i(20)}^{(q)} + \frac{1}{2}(3\xi^2 - 1)W_{i(02)}^{(q)}, \quad (7)$$

to complete the 2nd order polynomial representation, claiming that the cross-product terms are necessary in order “to achieve completeness and proper transition from the linear to the full quadratic order”. They justify this by reference to extensive finite-element literature, indicating that “improper transition can lead to undesirable effects such as gaps and overlaps between adjacent cells”. In making this argument, Haj-Ali and Aboudi neglect the fact that the choice of interpolation functions depends on the element shape which dictates whether a complete or incomplete polynomial is used. For instance, the extensively used Q4 and Q8 elements are indeed

based on incomplete polynomial representations of the displacement field, whereas a complete quadratic polynomial is employed for a six-noded triangular element. While the complete quadratic displacement field representation is necessary for displacement continuity between adjacent elements in the context of nodal-based triangular, but not quadrilateral, finite elements, it is neither necessary nor desirable in the context of the surface-averaging approach employed in the FVDAM theory based solely on the accepted conservation field equations and quadratic displacement field representation. Further, owing to the surface-averaging approach in imposing displacement (and traction) continuity conditions, the cross-product terms do not eliminate adjacent subvolume face interpenetration, rendering the main reason claimed by Haj-Ali and Aboudi for their inclusion, and hence extension of the parametric FVDAM theory, without justification. Hence the main argument for inclusion of the cross-product terms in the context of a surface-averaging approach is fundamentally flawed. Just as importantly, Haj-Ali and Aboudi (2010) do not substantiate the need for inclusion of these cross-product terms by demonstrating superior results relative to the already established parametric FVDAM theory based on the fluctuating displacement field representation of Eq. (3).

Moreover, the additional unknown coefficients require additional conditions, which Haj-Ali and Aboudi choose to be higher-order moments of the equilibrium equations,

$$\int_{V_{(q)}} y_2 y_3 \frac{\partial \sigma_{ji}^{(q)}}{\partial y_j} dV_{(q)} = \int_{S_{(q)}} y_2 y_3 t_i dS_{(q)} - \int_{V_{(q)}} (y_3 \sigma_{2i} + y_2 \sigma_{3i}) dV_{(q)} = 0, \quad (8)$$

where (y_2, y_3) are local coordinates with the origin placed at the subvolume's center. The introduction of the above equations is a drastic departure from the finite-volume approaches which are based solely on Eq. (5). Aside from the absence of any physical meaning of these equations, and therefore lack of connection with the satisfaction of conservation equations in the integral sense employed by the different variants of the finite-volume approaches, their use in determining the additional cross-product coefficients substantially limits the theoretical framework of the proposed extension of FVDAM, and leads to problems of which the potential user should be aware. First, the above equations are not coordinate-frame indifferent, producing different results for different choices of the local coordinate system (y_2, y_3) locations. Haj-Ali and Aboudi (2010) do indicate that these local coordinate systems are centered in the individual subvolumes which makes the theory coordinate-frame dependent. Nonetheless, there is no reason why the location of a coordinate system should play a critical role in a properly constructed theory. Moreover, these particular equations are identically satisfied for parametric mappings involving constant

Jacobians. As a consequence, the constant Jacobian approximation introduced by Cavalcante (2006) cannot be employed in a consistent manner, considerably slowing down the global stiffness matrix assembly. These problems are absent in the self-contained and internally-consistent parametric FVDAM approach.

As in the parametric FVDAM theory, Haj-Ali and Aboudi solve for the unknown coefficients $W_{i(-)}^{(q)}$ by enforcing traction and displacement continuity equations, and periodicity conditions, in a surface-average sense, albeit without constructing local stiffness matrices. The calculation of surface-average traction components requires numerical integration of certain terms due to the unstated requirement that variable Jacobians must be employed in light of Eq. (8). As discussed in the sequel, however, the use of variable Jacobian for mappings other than square, rectangular or parallelogram subvolumes leads to inconsistencies in the calculation of local stress averages based on the average stress theorem. Moreover, the additional “moment” equations may become ineffective for certain mappings when variable Jacobian is used if the coordinate system is not placed exactly at the subvolume centroid. These cases are discussed next.

3. Reducibility, coordinate frame indifference and self-consistency

The use of parametric mapping in conjunction with the cross-product terms in the subvolume displacement field representation employed by Haj-Ali and Aboudi does not always render the employed moment equations effective. Mappings involving subvolumes characterized by constant Jacobians lead to degenerate situations which violate the correct reducibility requirement of a consistent theoretical framework. Mappings characterized by variable Jacobians may also be identified which violate the coordinate frame indifference principle for small perturbations in the local coordinate system placement.

3.1. Mappings characterized by constant Jacobians

First, mapping of the square reference subvolume onto itself, a larger/smaller square or a rectangular subvolume, Fig. 2(a,b) automatically satisfies the newly introduced moment equations used to determine the cross-product coefficients. These mappings are characterized by constant Jacobians relating the partial derivatives of the reference (η, ξ) and physical $(y_2, y_3)^{(q)}$ coordinates. In this case, the HFGMC with arbitrary cell geometry reduces to that of the parametric FVDAM theory, but only when the cross-product coefficients are **manually** set to zero given that the moment equations are identically satisfied.

In particular, a consistently formulated theory must reduce correctly in the special case when the mapping is one-to-one, that is when the square reference subvolume is mapped onto itself. In this case, the unknown coefficients $W_{2(-)}^{(q)}$ are not obtained solely in terms of the surface-averaged displacements $\hat{u}_i^{(p)}$ as shown below for $E = 1000$ and $\nu = 1/3$

$$\begin{aligned} W_{2(00)}^{(q)} &= \frac{1}{2} \hat{u}_2^{(2)} + \frac{1}{2} \hat{u}_2^{(4)} - W_{2(20)}^{(q)}, \\ W_{2(10)}^{(q)} &= \frac{1}{2} \hat{u}_2^{(2)} - \frac{1}{2} \hat{u}_2^{(4)}, \\ W_{2(01)}^{(q)} &= -\frac{1}{2} \hat{u}_2^{(1)} + \frac{1}{2} \hat{u}_2^{(3)}, \\ W_{2(11)}^{(q)} &= -\frac{30}{13} \hat{u}_3^{(1)} + \frac{30}{13} \hat{u}_3^{(2)} - \frac{30}{13} \hat{u}_3^{(3)} + \frac{30}{13} \hat{u}_3^{(4)} - \frac{81}{13} W_{3(20)}^{(q)}, \\ W_{2(20)}^{(q)} &= W_{2(20)}^{(q)}, \\ W_{2(02)}^{(q)} &= \frac{1}{2} \hat{u}_2^{(1)} - \frac{1}{2} \hat{u}_2^{(2)} + \frac{1}{2} \hat{u}_2^{(3)} - \frac{1}{2} \hat{u}_2^{(4)} + W_{2(20)}^{(q)}, \end{aligned} \quad (9)$$

with similar expressions for $W_{3(-)}^{(q)}$. The additional moment equations are identically satisfied, and the satisfaction of the equilibrium equations in the surface-average sense does not automatically yield the result $W_{2(11)}^{(q)} = W_{3(11)}^{(q)} = 0$, as would be expected of a self-consistent theory.

A similar situation arises when the square reference subvolume is mapped onto a parallelogram in the actual microstructure, Fig. 2(c). This mapping is also characterized by constant Jacobian, reducing the HFGMC with arbitrary cell geometry to parametric FVDAM when the cross-product terms are manually set to zero. We note that in the cases involving constant Jacobians, the equilibrium equations are satisfied not only in an integral sense, but also point-wise, as discussed in more detail in the sequel. Our examination of the cases investigated by Haj-Ali and Aboudi lead us to believe that the authors did not allow the above situations to arise in discretizing the investigated unit cells. Nonetheless, the readers should be aware of the above problems. A practical consequence of the above flawed construction is the potential loss of linear independence of the global system of equations for the unknown coefficients $W_{i(-)}^{(q)}$ which may manifest itself as an ill-conditioned system, or a system with singular matrix.

3.2. Mappings characterized by variable Jacobians

For mappings that produce distorted subvolumes characterized by non-constant Jacobians, the moment equations employed by Haj-Ali and Aboudi provide a means of calculating the cross-product coefficients, notwithstanding the absence of physical meaning of these equations. However, these equations are local coordinate system specific and will produce different results when the local coordinate system is slightly perturbed. An example is provided in Fig. 2(d) where the reference subvolume is mapped onto a trapezoidal subvolume using the same material properties as in the first example. We consider two cases characterized by two sets of nodal coordinates of the mapped trapezoidal subvolume referred to slightly different local coordinate systems.

In the first case, the local coordinate system is placed directly at the subvolume's centroid yielding the following nodal coordinates $y_i^{(p,q)}$ ($i = 2, 3$): $(-1.1, -0.9841)$, $(1.1, -0.9841)$, $(1.0, 1.0159)$ and $(-1.0, 1.0159)$. When the Jacobian is taken as variable, the equilibrium equations yield the following relations,

$$\begin{aligned} \frac{10000a}{7} W_{3(10)}^{(q)} + \frac{12010500a}{91} W_{2(20)}^{(q)} + \frac{63000}{13} W_{2(02)}^{(q)} + 30000a W_{3(11)}^{(q)} &= 0, \\ \frac{10000a}{7} W_{2(10)}^{(q)} + \frac{4230000a}{91} W_{3(20)}^{(q)} + \frac{180000}{13} W_{3(02)}^{(q)} + 30000a W_{2(11)}^{(q)} &= 0, \end{aligned} \quad (10)$$

where $a = \ln 11 - \ln 5 - \ln 2$. Use of the additional moment equations given by Eq. (8), on the other hand, yields the following relations,

$$\begin{aligned} \frac{100}{2457} W_{2(10)}^{(q)} + \frac{100}{117} W_{2(11)}^{(q)} + \frac{2000}{441} W_{3(20)}^{(q)} &= 0, \\ \frac{2000}{441} W_{2(20)}^{(q)} + \frac{2000}{17199} W_{3(10)}^{(q)} + \frac{2000}{819} W_{3(11)}^{(q)} &= 0. \end{aligned} \quad (11)$$

Solving the above systems of equations, we obtain unique expressions for the coefficients $W_{i(-)}^{(q)}$ in terms of the surface-averaged displacements.

In the second case, the local coordinate system has its origin halfway between the horizontal and vertical coordinates of the 4 subvolume vertices, yielding a slightly different set of nodal coordinates: $(-1.1, -1.0)$, $(1.1, -1.0)$, $(1.0, 1.0)$ and $(-1.0, 1.0)$. When the Jacobian is taken as variable, the moment equations are identically satisfied, providing no additional means of evaluating the cross-product coefficients. Solving for the coefficients $W_{i(-)}^{(q)}$ using

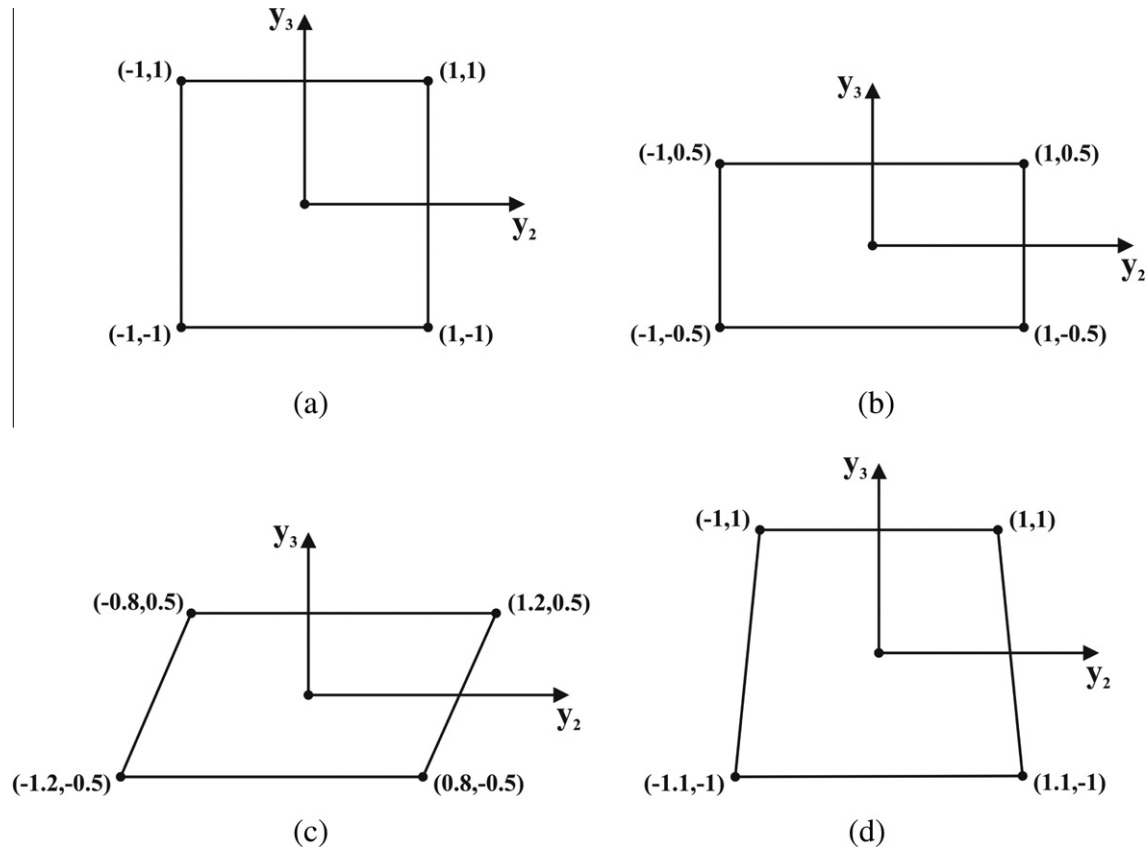


Fig. 2. Subvolumes mapped onto the actual microstructure of the unit cell for which the so-called moment equilibrium equations introduced by Haj-Ali and Aboudi (2010) are identically satisfied.

equilibrium equations satisfied in the surface-average sense, we obtain expressions similar to Eq. (9) in terms of the surface-averaged displacements and $W_{i(20)}^{(q)}$ ($i = 2, 3$) as free parameters. Upon manually setting the cross-product coefficients to zero one obtains the FVDAM theory equations.

The above trapezoidal subvolume example illustrates a fundamental flaw in the extension of the parametric FVDAM theory proposed by Haj-Ali and Aboudi, namely the violation of the frame indifference principle in general, and specifically in the presence of slight variations in the local coordinate system placement. In their article, Haj-Ali and Aboudi do not discuss the reason for their choice of local coordinate systems centered in each subvolume that are used in the implementation of the additional moment equations. This coordinate specific extension of the parametric FVDAM theory is a direct consequence of the introduction of additional equations which lack physical meaning, and hence which do not obey accepted mechanics principles.

In contrast, both the parametric homogenized (FVDAM) and structural finite-volume theories do not suffer from the above shortcomings. Specifically, one-to-one mapping produces the same equations for the displacement field coefficients as the original FVDAM theory based on rectangular unit cell discretization, i.e., proper reduction to the original model is obtained. Relaxation of the volume-averaged Jacobian approximation by its true expressions for general quadrilateral subvolume mappings also produces consistent theoretical and computational results. Moreover, the volume-averaged Jacobian simplification employed in the relations between the partial derivatives of displacement components in the reference and actual coordinates makes our finite-volume theories self-consistent as discussed below.

3.3. Average stress theorem

A key requirement of any homogenization theory is consistent averaging of the pertinent field variables in order to generate a consistent set of homogenized constitutive equations. While the parametric FVDAM theory meets this key requirement, the HFGMC with arbitrary cell geometry does not because the volume-averaged Jacobian simplification introduced originally by Cavalcante (2006) **cannot** be utilized in the solution for the unknown displacement field coefficients. This is rooted in the fundamental difference in satisfying the field equations in an integral and point-wise sense. Specifically, the average stress theorem states that, for an arbitrary body in equilibrium regardless of its composition, the average stress may be calculated from either the integral of the surface tractions or from the volume integral of the point-wise stresses. Denoting the average stress calculated from the surface traction by $\bar{\sigma}$, and by $\bar{\sigma}$ the volumetric average stress, we have

$$\begin{aligned}\bar{\sigma}_{ij} &= \frac{1}{V} \int_S t_i x_j dS = \frac{1}{V} \int_S \sigma_{ki} n_k x_j dS = \frac{1}{V} \int_V \frac{\partial}{\partial x_k} (\sigma_{ki} x_j) dV \\ &= \bar{\sigma}_{ij} + \frac{1}{V} \int_V \frac{\partial \sigma_{ki}}{\partial x_k} x_j dV.\end{aligned}\quad (12)$$

When the local equilibrium equations are satisfied in point-wise sense, i.e., $\partial \sigma_{ki} / \partial x_k = 0$, the above integral reduces to the standard definition for the volume-averaged stress. This is true for the FVDAM theory in the elastic region, owing to the employed quadratic displacement field and the use of the volume-averaged Jacobian in the displacement gradient relations. Specifically, the point-wise equilibrium equations in a quadrilateral subvolume generated by mapping given in Eq. (2) become

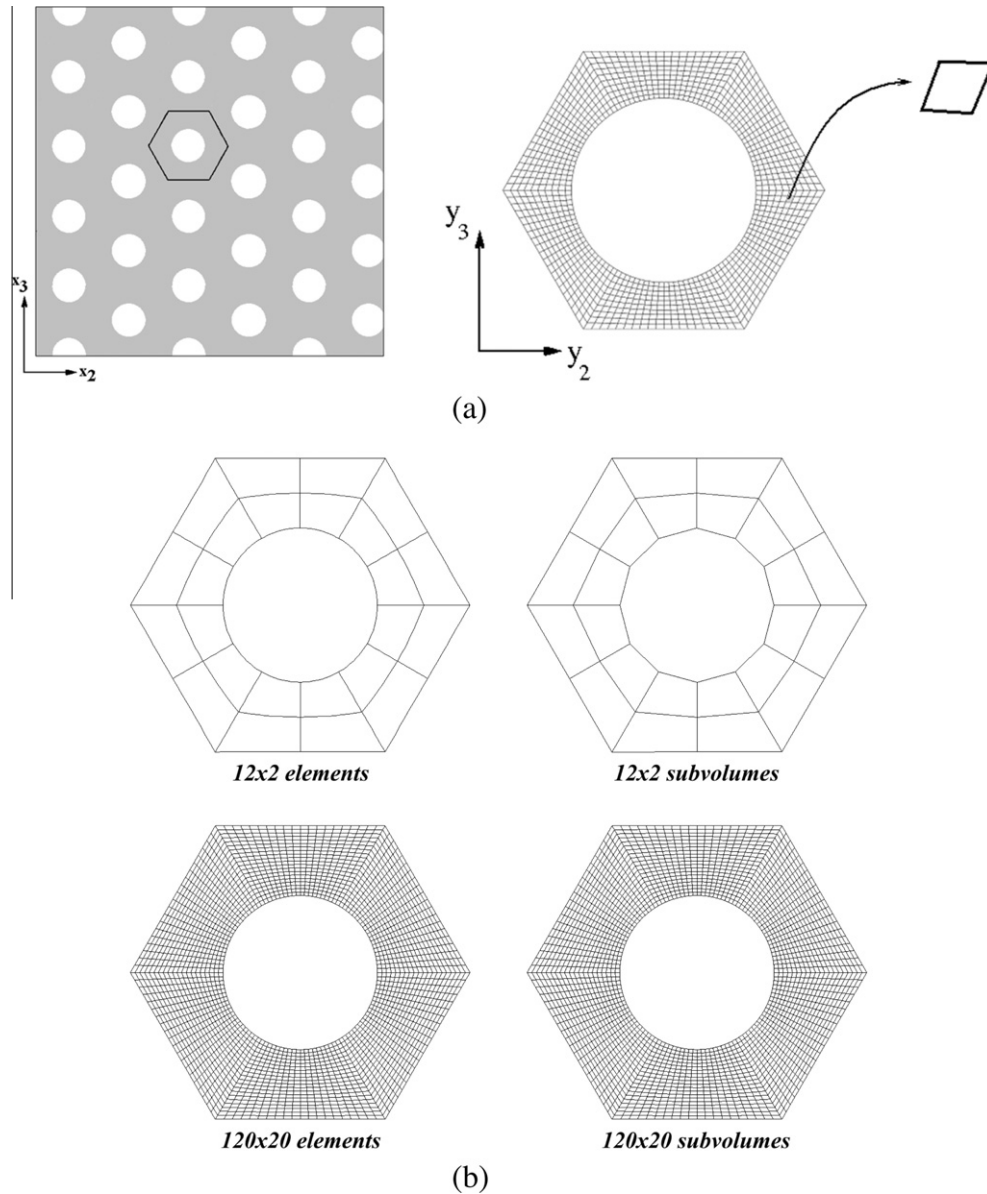


Fig. 3. (a) Hexagonal array of circular holes with a highlighted unit cell (left), and parametric FVDAM discretization of the unit cell using quadrilateral subvolumes (right); (b) mesh discretization ranges employed in the FEM (left) and FVDAM and HFGMC (right) simulations.

$$\frac{\partial \sigma_{ji}}{\partial x_j} = \frac{\partial \sigma_{ji}}{\partial \zeta_n} \frac{\partial \zeta_n}{\partial x_j} = 0,$$

where $(\zeta_2, \zeta_3) = (\eta, \xi)$. Given Hooke's law in the generalized form $\sigma_{ij} = C_{ijkl} \varepsilon_{kl}$ and the strain–displacement relations $\varepsilon_{kl} = 1/2(\partial u_k / \partial x_l + \partial u_l / \partial x_k)$, the Navier's equations become

$$C_{ijkl} \left(\frac{\partial^2 u_k}{\partial \zeta_n \partial \zeta_m} \frac{\partial \zeta_m}{\partial x_l} + \frac{\partial^2 u_l}{\partial \zeta_n \partial \zeta_m} \frac{\partial \zeta_m}{\partial x_k} \right) \frac{\partial \zeta_n}{\partial x_j} = 0.$$

Hence for a quadratic displacement field representation and constant Jacobian elements $\partial \zeta_m / \partial x_l$ and $\partial \zeta_m / \partial x_k$, the point-wise equilibrium equations reduce to terms involving coefficients associated with quadratic terms. In this case, the satisfaction of equilibrium equations in a point-wise and integral sense are equivalent. Alternatively, when the equilibrium equations are not satisfied in point-wise sense, the second term on the right handside of Eq. (12) will be generally non-zero.

In the case of the HFGMC with arbitrary cell geometry, the point-wise stress fields generally will not be self-equilibrating for mappings which produce variable Jacobians unless the simplification of volume-averaged Jacobian introduced by Cavalcante (2006) is utilized, rendering the additional moment equations without value. However, the use of variable Jacobians leads to two different values for the average subvolume, and thus homogenized, stresses that may be used in the construction of homogenized constitutive equations. The FVDAM theory does not suffer from this problem for **any** unit cell discretization when the fields are elastic.

4. Predictive capability of the parametric FVDAM and HFGMC theories vis-a-vis FEM

Haj-Ali and Aboudi (2010) characterize the construction of the parametric FVDAM theory with elastic–plastic phases by Khatam and Pindera (2009b) as an “attempt”. They ignore the original construction of the parametric FVDAM theory for strictly elastic

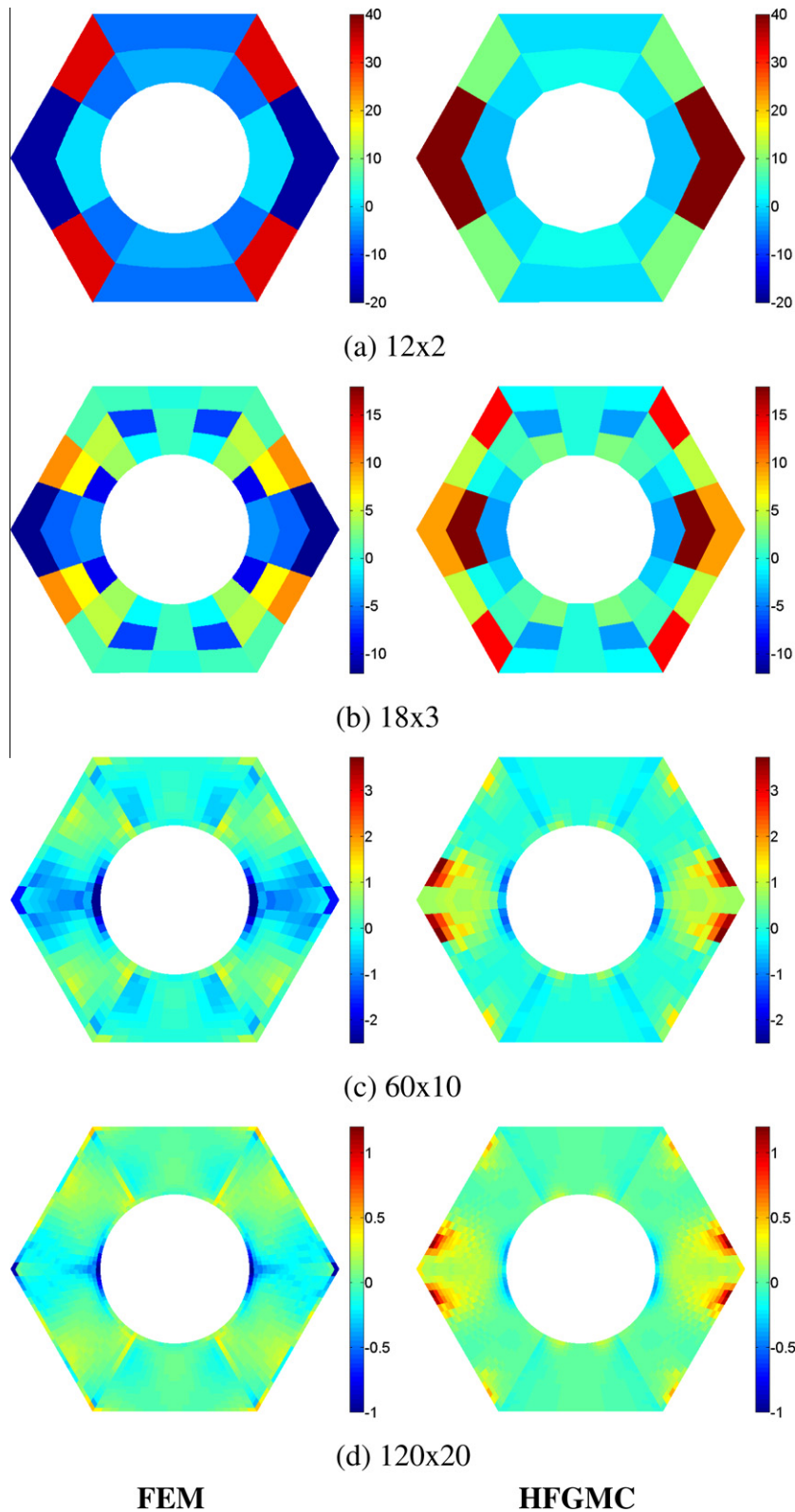


Fig. 4. Comparison of the normalized unbalanced average stress $\Delta\bar{\sigma}_{22}^q / \bar{\sigma}_{22}(\%)$ in unidirectionally loaded hexagonal array with 25% porosity by $\bar{\sigma}_{22} \neq 0$ at the homogenized strain $\bar{\epsilon}_{22} = 0.1\%$ for increasingly greater unit cell discretizations.

phases by Gattu et al. (2008), wherein its predictive capability to accurately capture local stress fields has been verified against the analytical solution for the Eshelby problem, which Haj-Ali and Aboudi (2010) duplicate in Fig. 4(a) and Fig. 5 of their own paper. They also ignore the documented predictive capability of the para-

metric FVDAM theory in the elastic–plastic domain illustrated in a sequence of papers dealing with a wide range of materials characterized by complex microstructures by Khatam and Pindera (2009a,b), Khatam et al. (2009) and Khatam and Pindera (2010, 2011), including verification with independently generated

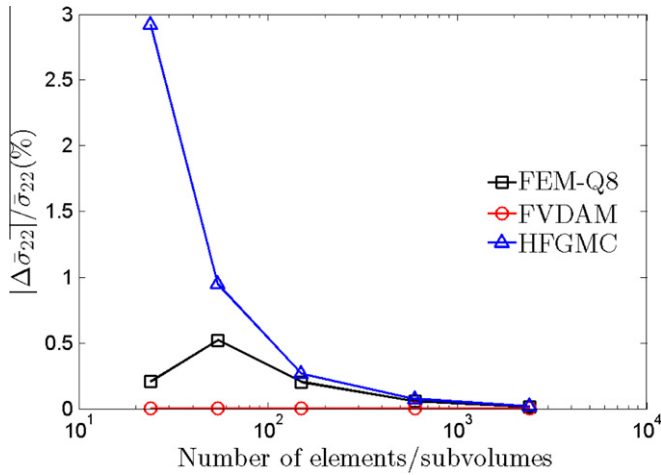


Fig. 5. Convergence of the unbalanced average stress $|\Delta\bar{\sigma}_{22}|/\bar{\sigma}_{22}$ (%) with mesh size at the homogenized strain level $\bar{\epsilon}_{22} = 0.1\%$ under loading by $\bar{\sigma}_{22} \neq 0$.

experimental results of Fedele et al. (2006) on perforated hexagonal arrays of circular holes.

Most recently, a thorough comparison of the parametric FVDAM theory with finite-element results of the elastic–plastic response for two different unit cell microstructures has been carried out by Cavalcante et al. (2011) for the first time on an equal footing. The analyzed unit cell architectures involved circular porosities in hexagonal arrays in plane stress, and wavy multilayers with different microstructural refinement in generalized plane strain. To accomplish this comparison on equal footing, a finite-element code has been developed that closely mimicked the solution framework based on elements of the homogenization theory employed in the FVDAM construction. This solution framework included the same overall two-scale displacement field representation (except for the fluctuating displacement component details), and application of the periodic boundary conditions. For the finite-element analysis, Q8 elements were used to ensure comparable displacement field approximation. The same number of quadrilateral subvolumes and Q8 elements were employed to discretize the unit cells, producing nearly the same vertex coordinates. The use of Q8 elements required numerical calculation of the local stiffness matrix elements, based on complete 9-point Gaussian quadrature, in contrast with the closed-form expressions developed for the parametric FVDAM framework. Both the FVDAM and finite-element codes have been written in MATLAB. This comparison demonstrated conclusively FVDAM's predictive capability.

In contrast, Haj-Ali and Aboudi (2010) never provide a justification for the inclusion of cross-product terms by showing that superior results are obtained relative to the parametric FVDAM predictions. To further demonstrate that the construction of the parametric FVDAM theory has indeed been successful without the need for the cross-product terms introduced by Haj-Ali and Aboudi (2010), we compare its predictive capability with the proposed HFGMC with arbitrary cell geometry and the finite-element method following the same approach employed in the most recent comparative study of Cavalcante et al. (2011). Towards this end, a MATLAB code was written based on the proposed theory of Haj-Ali and Aboudi (2010) to analyze the response of a hexagonal array of circular porosities in plane stress as a function of mesh discretization, Fig. 3, which simulates a thin perforated metallic sheet under inplane loading. The terms associated with variable Jacobians were evaluated numerically using the Newton–Cotes formula with 5×5 integration points, including subvolume vertices. As shown in the figure, hexagonal unit cells facilitate discretization based on trapezoidal elements or subvolumes (cells), thereby avoiding the

singularity issues with the proposed HFGMC theory discussed earlier. The analysis, limited to elastic phases, is based on the elastic constants $E = 72.7$ GPa and $\nu = 0.34$.

First, we investigate the local and global convergence of the HFGMC, FVDAM and finite-element solutions as a function of mesh refinement for a hexagonal array of circular holes with 25% porosity subjected to uniaxial loading by $\bar{\sigma}_{22} \neq 0$, with the remaining homogenized stresses equal to zero. Then, we compare the local stress fields, σ_{22} and σ_{23} for the employed meshes, as well as the deformed unit cell features in order to investigate the claim made by Haj-Ali and Aboudi (2010) regarding the need for the cross-product terms in order to ensure better adjacent subvolume conformability. This comparison is more demanding than the unit cells considered by Haj-Ali and Aboudi (2010), owing to the more complex geometry and thus more complicated periodic boundary conditions.

4.1. Average stress theorem and the homogenized response

In the case of the finite-element method, the local equilibrium equations are satisfied only in the limit with increasing mesh discretization, thereby allowing to define an unbalanced average stress in any subdomain of the unit cell based on Eq. (12) as follows

$$\Delta\bar{\sigma}_{ij} = \bar{\sigma}_{ij} - \bar{\sigma}_{ij} = \frac{1}{V} \int_S t_i x_j dS - \frac{1}{V} \int_V \sigma_{ij} dV. \quad (13)$$

At the element level, the unbalanced average stress components are calculated from the formula

$$\Delta\bar{\sigma}_{ij}|^q = (\bar{\sigma}_{ij} - \bar{\sigma}_{ij})^q = \frac{1}{V_q} \int_{S_q} t_i x_j|^q dS - \frac{1}{V_q} \int_{V_q} \sigma_{ij}|^q dV, \quad (14)$$

while for the entire domain of the unit cell, we have the formula

$$\Delta\bar{\sigma}_{ij} = \sum_{q=1}^N c_q \Delta\bar{\sigma}_{ij}|^q, \quad (15)$$

where $c_q = V_q/V$ is the volume fraction of the q th element or subvolume, and $V = \sum_{q=1}^N V_q$.

In the case of HFGMC with arbitrary cell geometry, the local equilibrium equations are not satisfied in a point-wise sense because the constant Jacobian approximation cannot be employed, allowing the use of the same measure. This is in contrast with the parametric FVDAM theory wherein the local equilibrium equations are satisfied point-wise, rendering the unbalanced average stress in any subvolume zero in the purely elastic domain.

To illustrate the degree to which local equilibrium is satisfied by the finite-element and HFGMC methods as a function of mesh refinement, Fig. 4 compares local distributions of the unbalanced average stress component $\Delta\bar{\sigma}_{22}|^q$ normalized by the average unit cell value $\bar{\sigma}_{22}$ for the four unit cell discretizations 12×2 , 18×3 , 60×10 and 120×20 at the applied strain level of $\bar{\epsilon}_{22} = 0.1\%$. The finite-element method is observed to exhibit superior performance to the proposed HFGMC with arbitrary cell geometry until sufficiently fine meshes are employed. Fig. 5 presents comparison of the global convergence characteristics of the HFGMC, FVDAM and finite-element methods, demonstrating that both the HFGMC and finite-element approaches are inferior to the parametric FVDAM theory based on the constant Jacobian approximation. The proposed HFGMC with arbitrary cell geometry is clearly inferior to the finite-element method, and requires substantial mesh refinement to produce results with the same fidelity as the finite-element method.

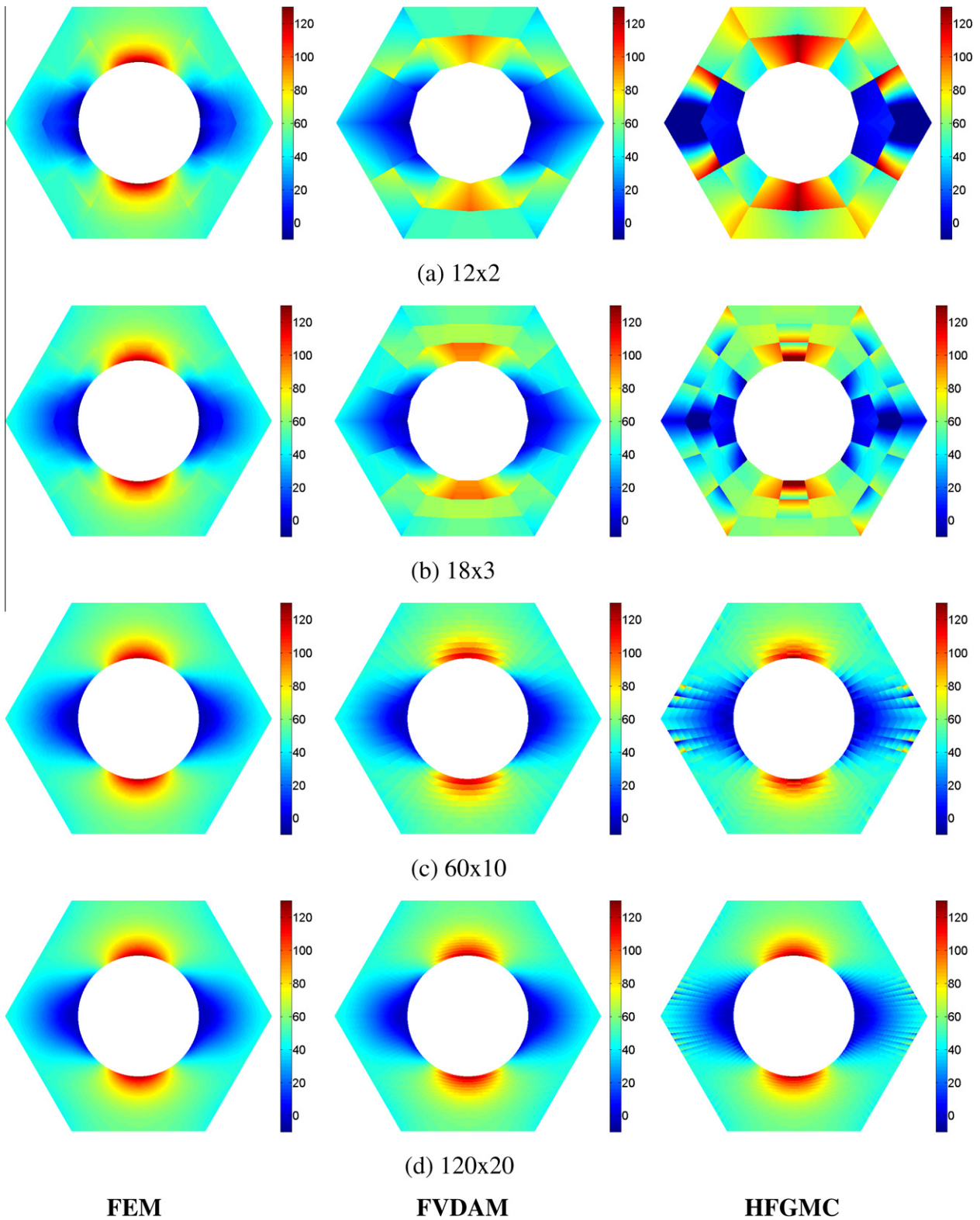


Fig. 6. Comparison of σ_{22} stress fields in unidirectionally loaded hexagonal array with 25% porosity by $\bar{\sigma}_{22} \neq 0$ at $\bar{\epsilon}_{22} = 0.1\%$ for increasingly greater unit cell discretizations.

4.2. Local stress fields

Fig. 6 presents comparison of local σ_{22} stress distributions generated at the applied strain level of $\bar{\epsilon}_{22} = 0.1\%$ by the finite-element and parametric FVDAM and HFGMC methods for increasingly re-

finer unit cells of the porous hexagonal array. While the stress distributions obtained from the parametric FVDAM theory take recognizable forms with as few as 12×2 subvolumes, comparing favorably with the corresponding finite-element calculations, considerably finer discretizations are required of the proposed

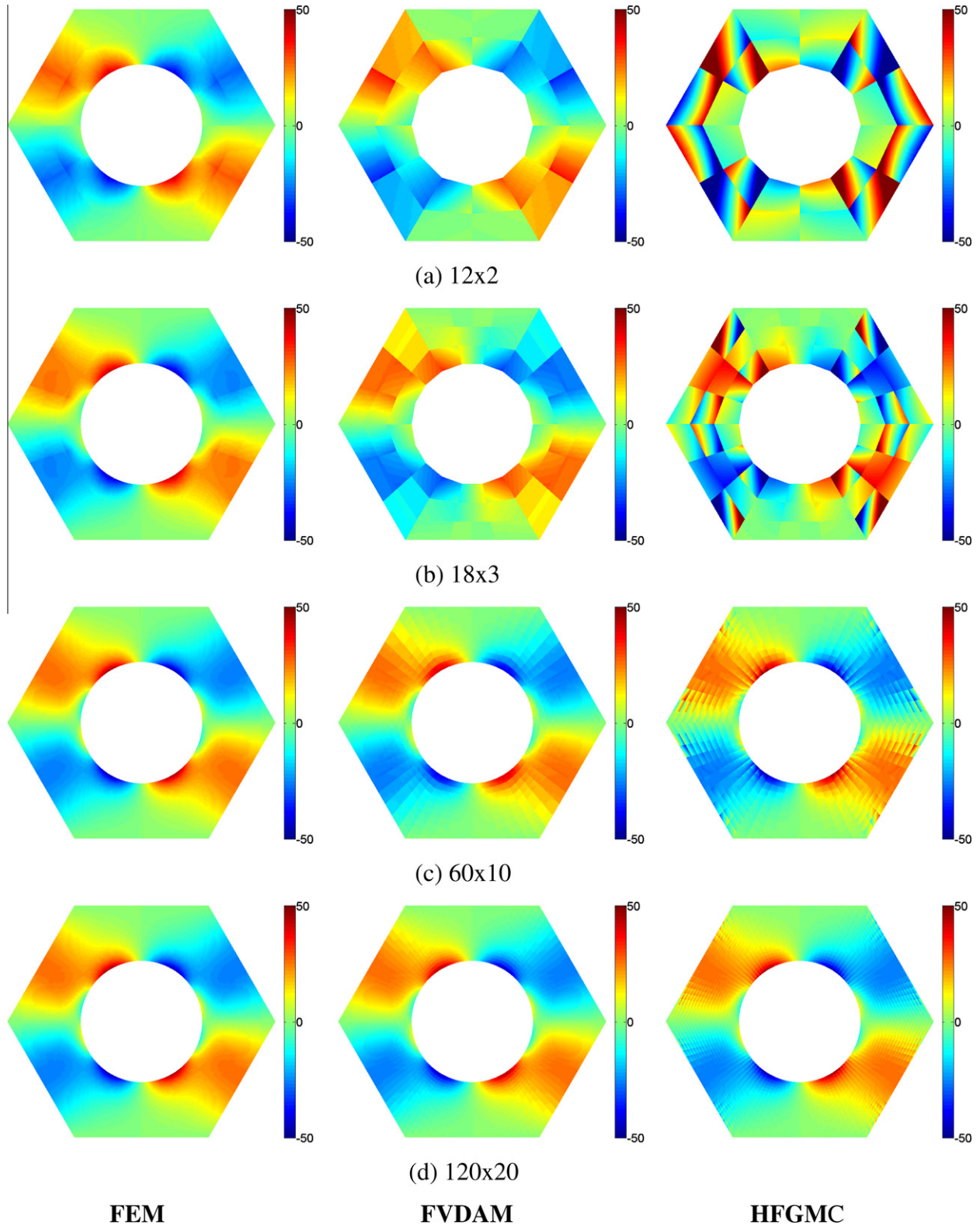


Fig. 7. Comparison of σ_{23} stress fields in unidirectionally loaded hexagonal array with 25% porosity by $\bar{\sigma}_{22} \neq 0$ at $\bar{\epsilon}_{22} = 0.1\%$ for increasingly greater unit cell discretizations.

HFGMC with arbitrary cell geometry. Even with the highest mesh discretization employed herein (120×20), the HFGMC σ_{22} distributions exhibit visible perturbations or discontinuities close to the unit cell boundaries subjected to uniaxial loading. Such perturbations are absent in the FVDAM predictions which are nearly indistinguishable from the finite-element results. Similar

observations hold for σ_{23} stress distributions shown in Fig. 7. The substantially greater stress field discontinuities observed in the HFGMC results relative to the FVDAM predictions suggest that the inclusion of cross-product terms does not produce the intended effect, namely better adjacent subvolume conformability. In fact, the opposite effect has been accomplished as illustrated next.

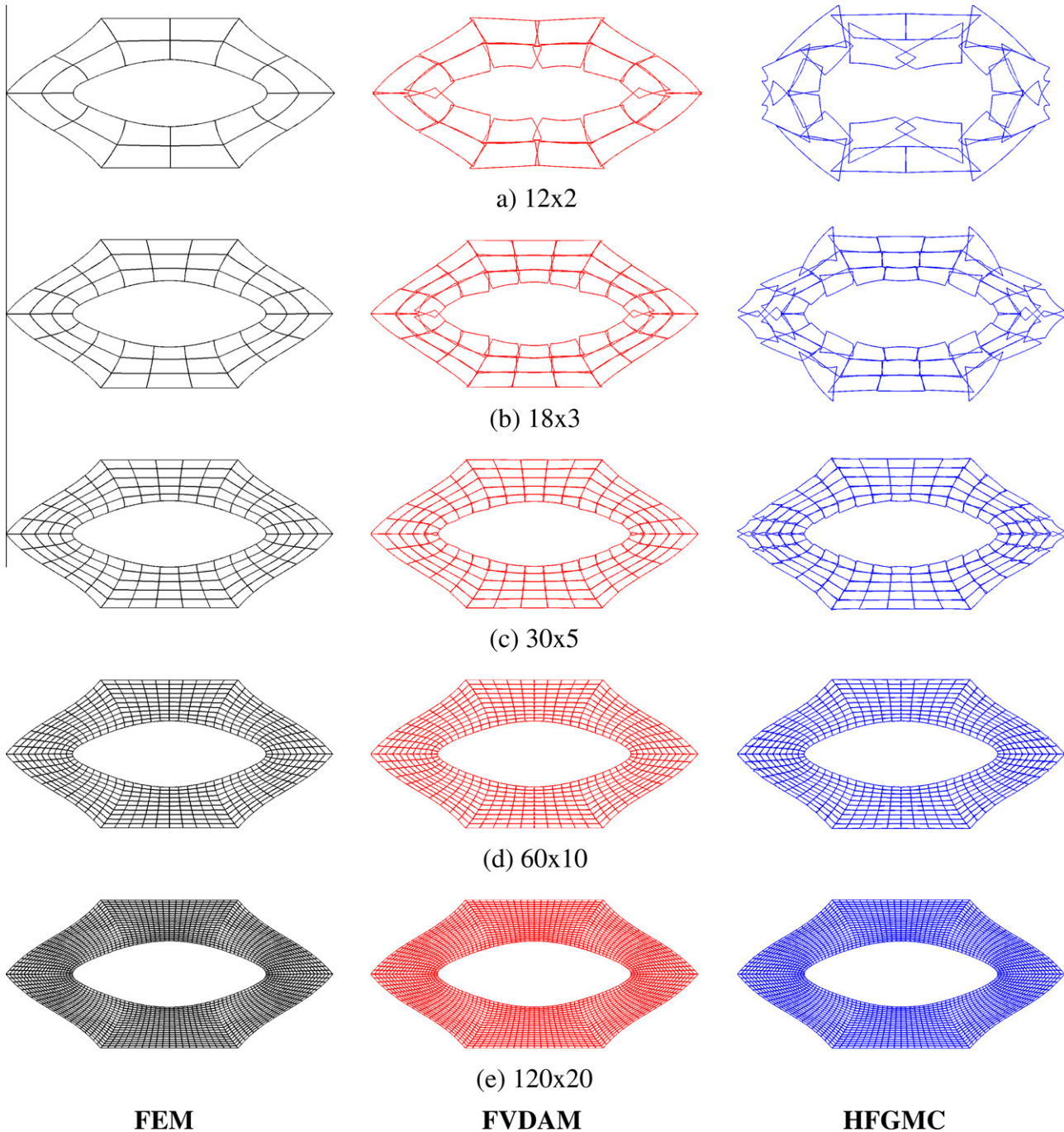


Fig. 8. Comparison of deformed meshes (magnified 500 times) of unidirectionally loaded hexagonal arrays with 25% porosity by $\bar{\sigma}_{22} \neq 0$ at $\bar{\varepsilon}_{22} = 0.1\%$ as a function of mesh refinement.

4.3. Point-wise interfacial displacement continuity

Fig. 8 compares unit cell deformations under the employed $\bar{\sigma}_{22} \neq 0$ loading at $\bar{\varepsilon}_{22} = 0.1\%$ for the five increasingly finer mesh discretizations. The Q8 elements employed in the finite-element calculations are conformable, ensuring displacement field continuity along adjacent element faces at each level of mesh discretization. In contrast, the interfacial displacement field continuity is satisfied only in a surface average sense in both parametric approaches, hence subvolume face rotations and concomitant interpenetrations are expected. Unfortunately, the additional cross-product terms in the quadratic displacement field representation substantially in-

crease the extent of face rotations predicted by HFGMC relative to the parametric FVDAM theory for small mesh discretizations, resulting in large adjacent interfacial interpenetrations and hence large unit cell distortions. These rotations are much smaller in the case of the parametric FVDAM theory and rapidly become negligibly small with increasing mesh refinement. For the 30×5 unit cell, the interpenetrations are not visually discernible, in contrast with the HFGMC results which exhibit substantial interfacial rotations of opposite sign for the boundary subvolumes subjected to the applied load. Clearly, the proposed HFGMC method requires substantially greater discretizations to achieve the same extent of interfacial conformability.

5. Discussion

In their article, Haj-Ali and Aboudi state that even though FVDAM is a direct implementation of HFGMC, Bansal and Pindera (2005, 2006) have changed its name to FVDAM. This characterization of the work by Bansal and Pindera, and the work discussed in the Introduction that followed, raises an interesting question of the circumstances and factors that justify name changes of theories, methods or approaches used in applied sciences, including applied mechanics. For instance, the distinction between finite-difference, finite-element and finite-volume techniques in the solution of governing field equations of mechanics or physics is clear. The reconstruction of the original higher-order theory for periodic multiphase materials of Aboudi et al. (2001) by Bansal and Pindera (2005, 2006) has clearly demonstrated that this approach belongs to the class of techniques called finite-volume methods, as summarized in Table 1. In contrast, re-naming the original higher-order theory for periodic multiphase materials as HFGMC by Aboudi et al. (2002) cannot be readily justified. As demonstrated by Bansal and Pindera (2006), while HFGMC is a displacement-based theory, GMC is fundamentally a stress-based model characterized by piece-wise uniform stress fields. Hence, fundamentally different asymptotic predictions are produced by the two methods with increasing/decreasing parameters which define unit cell microstructures, that may be completely erroneous in the presence of damage. Hence, there is no rational basis for connecting the two through similar names.

On the other hand, the extension of the parametric FVDAM by Haj-Ali and Aboudi (2010) through inclusion of cross-product terms in the quadratic displacement field approximation, and the concomitant introduction of additional moments of the equilibrium equations, suggest that the original name higher-order theory for periodic multiphase materials first introduced by Aboudi et al. (2001) may be more appropriate than HFGMC. Unfortunately, these additional moment equations employed within the parametric FVDAM framework based on single quadrilateral subvolumes and mapping introduced by Cavalcante (2006), as well as others in the context of the finite-volume method, produce an inconsistent theory which violates accepted mechanics principles.

6. Conclusions

In the IJSS manuscript titled "Formulation of the High-Fidelity Generalized Method of Cells with Arbitrary Cell Geometry for Refined Micromechanics and Damage in Composites" (Haj-Ali and Aboudi, 2010), the authors attempt to improve the well-established FVDAM theory by incorporating cross-product terms in the 2nd order displacement field representation at the local subvolume level. The formulation follows the framework of the parametric FVDAM theory, and not the original HFGMC construction as claimed, including the key parametric mapping concept also introduced by other researchers in the context of related finite-volume theories. The additional terms require additional equations for their determination. Haj-Ali and Aboudi propose to use certain moments of the equilibrium equations. These moments are not related to the moments of tractions well-understood in the mechanics community, thereby not only lacking physical basis but also leading to fundamental shortcomings at both theoretical and computational levels.

First, the additional equations are coordinate-frame dependent. To mitigate this shortcoming, Haj-Ali and Aboudi define the parametric mapping employed to generate quadrilateral subvolumes with respect to specific coordinate systems centered in each subvolume. Small deviations in the local coordinate system placement

will produce different systems of equations, and hence different solutions, including multiple solutions.

Second, the manner of defining these moment equations renders them without value for those parametric mappings which produce quadrilateral shapes characterized by constant Jacobians. In this case, the additional equations do not generate new information which would produce the needed linearly independent equations. **Manually** setting the cross-product term coefficients to zero in the resulting equations for the unknown displacement field coefficients reduces the proposed HFGMC model to the well-established FVDAM theory. Otherwise, multiple solutions are obtained. A practical consequence is the potential loss of linear independence of the global system of equations for the unknown coefficients $W_{i(\cdot)}^{(q)}$ which may manifest itself as an ill-conditioned system, or a system with singular matrix.

For those mappings which leverage the additional moment equations, the local equilibrium equations are not satisfied in a point-wise sense. Hence, the Average Stress Theorem for heterogeneous materials is violated for insufficiently fine unit cell discretizations, with concomitant consequence for the construction of homogenized constitutive equations. Moreover, the manner in which the additional equations have been defined eliminates the possibility of substantially accelerating the model's execution times by approximating the parametric coordinate transformation Jacobian by its volume-averaged value for those subvolume mappings characterized by variable Jacobians. This is important for unit cell microstructures requiring refined meshes.

Finally, direct comparison of the results generated using the proposed HFGMC approach with the finite-element method and the parametric FVDAM theory on an equal footing demonstrated the inferior predictive capability of Haj-Ali and Aboudi's method. In fact, the authors' attempt to improve the parametric FVDAM theory's predictive capability in the proposed manner had the opposite effect, clearly seen in the enhanced interpenetration of adjacent subvolume faces.

References

- Aboudi, J., Pindera, M.-J., Arnold, S.M., 1999. Higher-order theory for functionally graded materials. *Comp. B* 30 (8), 777–832.
- Aboudi, J., Pindera, M.-J., Arnold, S.M., 2001. Linear thermoelastic higher-order theory for periodic multiphase materials. *J. Appl. Mech.* 68 (5), 697–707.
- Aboudi, J., Pindera, M.-J., Arnold, S.M., 2002. High-fidelity generalized method of cells for inelastic periodic multiphase materials. NASA Technical Memorandum 2002-211469, NASA-Glenn Research Center, Cleveland, OH. March 2002.
- Achenbach, J.D., 1975. *A Theory of Elasticity with Microstructure for Directionally Reinforced Composites*. Springer-Verlag, New York.
- Bailey, C., Cross, M., 1995. A finite volume procedure to solve elastic solid mechanics problems in three dimensions on an unstructured mesh. *Int. J. Numer. Methods Eng.* 38, 1757–1776.
- Bansal, Y., Pindera, M.-J., 2003. Efficient reformulation of the thermoelastic higher-order theory for fgms. *J. Therm. Stresses* 26 (11–12), 1055–1092.
- Bansal, Y., Pindera, M.-J., 2005. A second look at the higher-order theory for periodic multiphase materials. *J. Appl. Mech.* 72, 177–195. See also: NASA CR2004-213043.
- Bansal, Y., Pindera, M.-J., 2006. Finite-volume direct averaging micromechanics of heterogeneous materials with elastic-plastic phases. *Int. J. Plast.* 22 (5), 775–825.
- Basic, H., Demirdzic, I., Muzaferija, S., 2005. Finite volume method for simulation of extrusion processes. *Int. J. Numer. Methods Eng.* 62, 475–494.
- Bijelonja, I., Demirdzic, I., Muzaferija, S., 2006. A finite volume method for incompressible linear elasticity. *Comput. Methods Appl. Mech. Eng.* 195, 6378–6390.
- Cavalcante, M.A.A., 2006. Modelling of the transient thermo-mechanical behavior of composite material structures by the finite-volume theory, MS Thesis, Federal University of Alagoas, Maceio, Alagoas, Brazil.
- Cavalcante, M.A.A., Marques, S.P.C., Pindera, M.-J., 2007a. Parametric formulation of the finite-volume theory for functionally graded materials. Part I: Anal. *J. Appl. Mech.* 74 (5), 935–945.
- Cavalcante, M.A.A., Marques, S.P.C., Pindera, M.-J., 2007b. Parametric formulation of the finite-volume theory for functionally graded materials. Part II: Numer. Results. *J. Appl. Mech.* 74 (5), 946–957.

- Cavalcante, M.A.A., Marques, S.P.C., Pindera, M.-J., 2008. Computational aspects of the parametric finite-volume theory for functionally graded materials. *J. Comput. Mater. Sci.* 44, 422–438.
- Cavalcante, M.A.A., Marques, S.P.C., Pindera, M.-J., 2009. Transient thermo-mechanical analysis of a layered cylinder by the parametric finite-volume theory. *J. Therm. Stresses* 32 (1), 112–134.
- Cavalcante, M.A.A., Khatam, H., Pindera, M.-J., 2011. Homogenization of elastic-plastic periodic materials by FVDAM and FE approaches –an assesment. *Comp. Part B* 42, 1713–1730.
- Demirdzic, I., Martinovic, D., Ivankovic, A., 1988. Numerical simulation of thermomechanical deformation processes in a welded work-piece. *Zavarivanje* 31, 209–219, in Serbo-Croat.
- Demirdzic, I., Martinovic, D., 1993. Finite volume method for thermo-elastic-plastic stress analysis. *Comput. Methods Appl. Mech. Eng.* 109, 331–349.
- Demirdzic, I., Muzafertija, S., 1994. Finite volume method for stress analysis in complex domains. *Int. J. Numer. Methods Eng.* 37, 3751–3766.
- Fallah, N., 2004. A cell vertex and cell centred finite volume method for plate bending analysis. *Comput. Methods Appl. Mech. Eng.* 193, 3457–3470.
- Fallah, N., 2005a. A new approach in cell centred finite volume formulation for plate bending analysis. *Lect. Ser. Comput. Comput. Sci.* 4, 187–190.
- Fallah, N., 2005b. Using shape function in cell centred finite volume formulation for two dimensional stress analysis. *Lect. Ser. Comput. Comput. Sci.* 4, 183–186.
- Fallah, N., 2006. On the use of shape functions in the cell centered finite volume formulation for plate bending analysis based on Mindlin–Reissner plate theory. *Comput. Struct.* 84, 1664–1672.
- Fallah, N., 2008. A method for the calculation of face gradients in the two-dimensional, cell centred, finite volume formulation for stress analysis in solid problems. *Scientia Iranica (Int. J. Sci. Tech.)* 15 (3), 286–294.
- Fedele, R., Maier, G., Whelan, M., 2006. Stochastic calibration of local constitutive models through measurements at the macroscale in heterogeneous media. *Comput. Methods Appl. Mech. Eng.* 195, 4971–4990.
- Fryer, Y.D., Bailey, C., Cross, M., Lai, C.-H., 1991. A control volume procedure for solving the elastic stress-strain equations on an unstructured mesh. *Appl. Math. Model.* 15, 639–645.
- Gao, X., Song, Y., Sun, Z., 2009. Quadrilateral subcell based finite volume micromechanics theory for multiscale analysis of elastic periodic materials. *J. Appl. Mech.* 76, 011013–1.
- Gattu, M., Khatam, H., Drago, A.S., Pindera, M.-J., 2008. Parametric finite-volume micromechanics of uniaxial, continuously-reinforced periodic materials with elastic phases. *J. Eng. Math. Tech.* 130 (3), 31015–15.
- Haj-Ali, R., Aboudi, J., 2010. Formulation of the high-fidelity generalized method of cells with arbitrary cell geometry for refined micromechanics and damage in composites. *Int. J. Solids Struct.* 47, 3447–3461.
- Khatam, H., Pindera, M.-J., 2009a. Thermo-elastic moduli of periodic multilayers with wavy architectures. *Composites B* 40 (1), 50–64.
- Khatam, H., Pindera, M.-J., 2009b. Parametric finite-volume micromechanics of periodic materials with elastoplastic phases. *Int. J. Plast.* 25 (7), 1386–1411.
- Khatam, H., Chen, L., Pindera, M.-J., 2009. Elastic and plastic response of perforated metal sheets with different porosity architectures. *J. Eng. Mat. Tech.* 131 (3), 031015–14.
- Khatam, H., Pindera, M.-J., 2010. Plasticity-triggered architectural effects in periodic multilayers with wavy microstructures. *Int. J. Plast.* 26 (2), 273–287.
- Khatam, H., Pindera, M.-J., 2011. Plastic deformation modes in perforated sheets and their relation to yield and limit surfaces. *Int. J. Plast.* 27 (10), 1537–1559.
- Paley, M., Aboudi, J., 1992. Micromechanical analysis of composites by the generalized method of cells model. *Mech. Mater.* 14, 127–139.
- Pan, W., Wheel, M.A., Qin, Y., 2010. Six-node triangle finite volume method for solids with a rotational degree of freedom for incompressible material. *Comput. Struct.* 88, 1506–1511.
- Taylor, G.A., Bailey, C., Cross, M., 1995. Solutions of the elastic/visco-plastic constitutive equations: a finite volume approach. *Appl. Math. Model.* 19, 746–760.
- Taylor, G.A., Bailey, C., Cross, M., 2003. A vertex-based finite volume method applied to non-linear material problems in computational solid mechanics. *Int. J. Numer. Methods Eng.* 56, 507–529.
- Versteeg, H.K., Malalasekera, W., 1995. *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*. Prentice Hall, New York.
- Wheel, M.A., 1996. A finite-volume approach to the stress analysis of pressurized axisymmetric structures. *Int. J. Press. Vessels Piping* 68, 311–317.
- Wenke, P., Wheel, M.A., 2003. A finite volume method for solid mechanics incorporating rotational degrees of freedom. *Comput. Struct.* 81, 321–329.
- Wheel, M.A., 2008. A control volume-based finite element method for plane micropolar elasticity. *Int. J. Numer. Methods Eng.* 75, 992–1006.
- Zhong, Y., Bansal, Y., Pindera, M.-J., 2004. Efficient reformulation of the thermal higher-order theory for FGM's with variable thermal conductivity. *Int. J. Comput. Eng. Sci.* 5 (4), 795–831, See also: NASA CR 2002–211910, November 2002.